Validity of Quantum Adiabatic Theorem

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Abstract
The consistency of quantum adiabatic theorem has been doubted recently. It is shown in the present paper, that the difference between the adiabatic solution and the exact solution to the Schrödinger equation with a slowly changing driving Hamiltonian is small; while the difference between their time derivatives is not small. This explains why substituting the adiabatic solution back into Schrödinger equation leads to ‘inconsistency’ of the adiabatic theorem. Physics is determined completely by the state vector, and not by its time derivative. Therefore the quantum adiabatic theorem is physically correct.

0.1 Introduction
Quantum adiabatic theorem (QAT) dates back to the early years of quantum mechanics[1]. It has important applications within and beyond quantum physics. In 1984, M. Berry found there is a geometrical phase in the adiabatically evolving wavefunction besides the dynamic phase[2]. B. Simon pointed out Berry’s phase factor is the holonomy of a Hermitian line bundle[3]. This started a rush for geometrical phases in quantum physics[4], which helped people to get deeper insight into many physical phenomena, such as Bohm-Aharanov effect, quantum Hall effect, etc. Recently, the quantum adiabatic theorem has renewed its importance in the context of quantum control and quantum computation[5]. More recently, however, the consistency of QAT has been doubted[6]. In their paper entitled "Inconsistency in the application of the adiabatic theorem", K.-P. Marzlin and B.C. Sanders gave a proof of inconsistency of QAT, and declared that the standard treatment of QAT alone does not ensure that a formal application of it result in correct results. This interesting suggestion has attracted attention from the physics circle[7]. The purpose of this letter is to point out that the QAT does give approximate state-vectors (wavefunctions), but not necessarily the approximate time derivatives of state-vectors. While physics is completely determined by the state-vector, and has nothing to do with its time derivative. Therefore the QAT is physically correct. What leads to ‘inconsistency’ of the QAT is neglecting the fact that the adiabatic approximate state-vector does not necessarily give the approximate time derivative of
state-vector \(\|\psi_A(t) - \psi(t)\| \ll 1 \Rightarrow \|\dot{\psi}_A(t) - \dot{\psi}(t)\| \ll 1\), where \(\|\varphi\| \equiv \sqrt{\langle \varphi|\varphi\rangle}\) denotes the norm of state-vector \(\varphi\).

0.2 Standard treatment of QAT

Suppose that the Hamiltonian depends on \(N\) real parameters \(R^1, \ldots, R^N:\)

\[H = H(R^1, \ldots, R^N) = H(R)\] (1)

When the representing point of the Hamiltonian describes slowly a finite curve \(C\) on the \(N\)-dimensional parameter manifold \(\mathcal{M}\)

\[C : R^\sigma = R^\sigma(t), \forall t \in [0, T], 1 \leq \sigma \leq N\] (2)

where \(T\) is the evolution time, let us study the evolution of the system. The instantaneous Hamiltonian’s eigen equation is

\[H(R)u_n(R) = E_n(R)u_n(R)\] (3)

Getting to the rotating representation

\[\psi(t) = \sum_{n \geq 0} c_n(t)u_n(R(t)) \exp\left[\frac{-i}{\hbar} \int_0^t E_n(R(t')) dt'\right]\] (4)

we get the Schrödinger equation

\[\dot{c}_m(t) = -\sum_{n \geq 0} \left\langle u_m(R(t)) \mid \dot{u}_n(R(t))\right\rangle \times \exp\left\{\frac{i}{\hbar} \int_0^t [E_m(R(t')) - E_n(R(t'))] dt'\right\} c_n(t)\] (5)

To avoid confusion of infinitesimals of different orders and to show what ‘rapidly oscillating’ means, let’s change to the dimensionless time \(\tau = t/T\)

\[\frac{d}{d\tau}\tilde{c}_m(\tau) = -\sum_{n \geq 0} \left\langle u_m(\tilde{R}(\tau)) \mid \frac{d}{d\tau}u_n(\tilde{R}(\tau))\right\rangle \times \exp\left\{\frac{i}{\hbar} T \int_0^\tau [E_m(\tilde{R}(\tau')) - E_n(\tilde{R}(\tau'))] d\tau'\right\} \tilde{c}_n(\tau)\] (6)

where

\[\tilde{c}_m(\tau) = c_m(T\tau) = c_m(t), \tilde{R}(\tau) = R(T\tau) = R(t)\] (7)

The initial value problem of the above differential equations is equivalent to the following integral equations

\[\tilde{c}_m(\tau) = \tilde{c}_m(0) - \sum_{n \geq 0} \int_0^\tau \left\langle u_m(\tilde{R}(\tau_1)) \mid \frac{d}{d\tau}u_n(\tilde{R}(\tau_1))\right\rangle \times \exp\left\{\frac{i}{\hbar} T \int_0^{\tau_1} [E_m(\tilde{R}(\tau')) - E_n(\tilde{R}(\tau'))] d\tau'\right\} \tilde{c}_n(\tau_1)d\tau_1\] (8)
Let’s slow down evenly the changing speed of the Hamiltonian while keep the finite curve $C$ fixed. Mathematically, that is to let $T \to \infty$, while keeping the function form of $\dot{R}(\tau)$ unchanged. The oscillating factors in the integrand ensure vanishing of the corresponding integrals. There is no resonance problem in the mathematical context. For the practical physical problem, slowly changing of the Hamiltonian means $T$ is such a long time that
\[
\left| \frac{\langle u_m(R(t)) \mid \dot{u}_n(R(t)) \rangle}{E_m(R(t)) - E_n(R(t))} \right| \ll 1 \tag{9}
\]
In both mathematics and physics contexts, the integral equation (8) can be approximately rewritten as
\[
\dot{c}_m^A(\tau) = \dot{c}_m(0) - \int_0^\tau \left\langle u_m(R(\tau_1)) \mid \frac{d}{d\tau} u_m(R(\tau_1)) \right\rangle \dot{c}_m^A(\tau_1)d\tau_1 \tag{10}
\]
Solving this equation by using iteration gives
\[
\dot{c}_m^A(\tau) = \exp \left\{ -\int_0^\tau \left\langle u_m(R(\tau_1)) \mid \frac{d}{d\tau} u_m(R(\tau_1)) \right\rangle d\tau_1 \right\} \dot{c}_m(0) \tag{11}
\]
This proves the QAT.

### 0.3 Analysis of ‘Inconsistency’ of QAT

When we substitute the adiabatic approximate solution (11) back into the integral equations (8), the equations approximately hold.
\[
0 \approx -\sum_{n(\neq m)} \left\langle u_m(R(\tau)) \mid \frac{d}{d\tau} u_n(R(\tau)) \right\rangle \times 
\exp \left\{ \frac{i}{\hbar} T \int_0^\tau \left[ E_m(\dot{R}(\tau')) - E_n(\dot{R}(\tau')) \right] d\tau' \right\} \dot{c}_n^A(\tau_1)d\tau_1 \tag{12}
\]
However, when we substitute the adiabatic approximate solution (11) back into the differential equations (6) whose initial value problem is equivalent to the integral equations (8), we obtain
\[
0 \approx -\sum_{n(\neq m)} \left\langle u_m(R(\tau)) \mid \frac{d}{d\tau} u_n(R(\tau)) \right\rangle \times 
\exp \left\{ \frac{i}{\hbar} T \int_0^\tau \left[ E_m(\dot{R}(\tau')) - E_n(\dot{R}(\tau')) \right] d\tau' \right\} \dot{c}_n^A(\tau) \tag{13}
\]
Considering that $\psi(0)$ can be an arbitrary state-vector, we have
\[
0 \approx \left\langle u_m(R(\tau)) \mid \frac{d}{d\tau} u_n(R(\tau)) \right\rangle, \forall m \neq n \tag{14}
\]
which is false. Notice that the right-hand side of (13) is the derivative of the right-hand side of (12), while (12) is correct and (13) is incorrect. In order to
understand the situation we are facing, let’s study the following basic mathematical fact. Let \( |\psi(t)\rangle \equiv |0\rangle e^{-i\omega t} + \varepsilon |1\rangle e^{-it/(\varepsilon^2)} \), \( (0 < \varepsilon \ll 1) \), \( |\varphi(t)\rangle \equiv |0\rangle e^{-i\omega t} \), where \( |0\rangle, |1\rangle \) are eigen vectors of the 1-dimensional harmonic oscillator energy.

\[
\therefore ||\psi(t) - \varphi(t)|| = \varepsilon \ll 1, \therefore |\psi(t)\rangle \approx |\varphi(t)\rangle \tag{15}
\]

While

\[
\therefore \left\| \dot{\psi}(t) - \dot{\varphi}(t) \right\| = 1/\varepsilon \gg 1, \therefore |\dot{\psi}(t)\rangle \approx |\dot{\varphi}(t)\rangle \tag{16}
\]

The above example shows that two approximately equal time-dependent state-vectors do not necessarily have approximately equal time derivatives. Therefore the approximate solution to integral equations (8) does not ensure that the equivalent differential equations (6) approximately hold. It is neglect of this basic mathematical fact that leads to ‘Inconsistency’ of QAT in [6].

QAT gives the approximate state-vector, not the approximate time derivative of the state-vector. All the physics is, however, determined by the state-vector itself, not by its time derivative. Therefore QAT is completely correct physically.

### 0.4 An exactly solvable example

Let’s consider an exactly solvable example, the evolution of the spin wavefunction of an electron in a slowly rotating magnetic field \( \vec{B}(t) = B_0 \left( i \cos \frac{2\pi}{T} t + j \sin \frac{2\pi}{T} t \right) \). The instantaneous Hamiltonian is

\[
H(t) = -\vec{\mu} \cdot \vec{B}(t) = \frac{e}{m} \vec{\sigma} \cdot \vec{B}(t) = \frac{\epsilon h}{2m} \vec{\sigma} \cdot \vec{B}(t)
\]

\[
= \frac{\epsilon h B_0}{2m} \begin{bmatrix} 0 & e^{-i\pi t/T} \\ e^{i\pi t/T} & 0 \end{bmatrix}
= \varepsilon \begin{bmatrix} 0 & e^{-i\pi t/T} \\ e^{i\pi t/T} & 0 \end{bmatrix}
\tag{17}
\]

Its eigenvalues are \( E_{\pm}(t) = \pm \varepsilon \). And the corresponding eigenvectors are

\[
u_{\pm}(t) = \frac{1}{\sqrt{2}} \begin{bmatrix} e^{-i\pi t/T} \\ \pm e^{i\pi t/T} \end{bmatrix}
\tag{18}
\]

The exact general solution to the Schrodinger equation

\[
\dot{i}h \frac{d}{dt} \psi(t) = H(t) \psi(t)
\tag{19}
\]

or

\[
\dot{i}h \frac{d}{dt} \begin{bmatrix} x(t) \\ y(t) \end{bmatrix} = \varepsilon \begin{bmatrix} 0 & e^{-i\pi t/T} \\ e^{i\pi t/T} & 0 \end{bmatrix} \begin{bmatrix} x(t) \\ y(t) \end{bmatrix}
\tag{20}
\]

is

\[
\psi(t) = \begin{bmatrix} x(t) \\ y(t) \end{bmatrix} = \begin{bmatrix} \frac{1}{A^2} [c_1(B+C)e^{iCt} + c_2(B-C)e^{-iCt}]e^{-iBt} \\ [c_1 e^{iCt} + c_2 e^{-iCt}]e^{iBt} \end{bmatrix}
\tag{21}
\]
where $A = \varepsilon / \hbar, B = \pi / T, C = \sqrt{A^2 + B^2}$, and $c_1, c_2$ are the integral constants. The specific solution determined by the initial condition

$$\psi(0) = \begin{bmatrix} x(0) \\ y(0) \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

is

$$\psi(t) = \frac{1}{\sqrt{2}} \begin{bmatrix} (\cos Ct - i \frac{A-B}{C} \sin Ct) e^{-iBt} \\ (\cos Ct - i \frac{A+B}{C} \sin Ct) e^{iBt} \end{bmatrix}$$

(23)

Let’s get into the rotating representation.

$$\psi(t) = c_+ (t) u_+ (t) e^{-itA} + c_- (t) u_- (t) e^{itA}$$

(24)

The exact Schrödinger equation becomes

$$\hat{c}_+ (t) = iB e^{i2At} c_- (t)$$

$$\hat{c}_- (t) = iB e^{-i2At} c_+ (t)$$

(25)

Its general solution is

$$\begin{bmatrix} c_+ (t) \\ c_- (t) \end{bmatrix} = \begin{bmatrix} e^{iAt} \left( \frac{C-A}{iB} c'e^{iCt} - \frac{C+A}{iB} c''e^{-iCt} \right) \\ e^{-iAt} \left( c'e^{iCt} + c''e^{-iCt} \right) \end{bmatrix}$$

(26)

The specific solution determined by the initial condition

$$\begin{bmatrix} c_+ (0) \\ c_- (0) \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

(27)

is

$$\begin{bmatrix} c_+ (t) \\ c_- (t) \end{bmatrix} = \begin{bmatrix} (\cos Ct - i \frac{A}{B} \sin Ct) e^{iAt} \\ (i \frac{B}{C} \sin Ct) e^{-iAt} \end{bmatrix}$$

(28)

The adiabatic approximation means neglecting the non-diagonal ($n \neq m$) terms, which contain oscillating factors, on the right-hand side of differential equations (25). The adiabatic approximate solution determined by the initial condition (27) is

$$\begin{bmatrix} c^A_+ (t) \\ c^A_- (t) \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

(29)

Getting to the dimensionless time $\tau = t/T$, we rewrite (28) and (29) as

$$\begin{bmatrix} \hat{c}_+ (\tau) \\ \hat{c}_- (\tau) \end{bmatrix} =$$

$$\begin{bmatrix} \left( \cos \sqrt{\frac{\varepsilon T}{\hbar}} + \frac{\pi^2}{2} - i \frac{\varepsilon T}{\hbar} \sin \sqrt{\left( \frac{\varepsilon T}{\hbar} \right)^2 + \pi^2} \right) e^{i\varepsilon T\tau / \hbar} \\ \left( i \frac{\varepsilon T}{\hbar} \sin \sqrt{\left( \frac{\varepsilon T}{\hbar} \right)^2 + \pi^2} \right) e^{-i\varepsilon T\tau / \hbar} \end{bmatrix}$$

(30)
It’s easy to see that
\[
\begin{bmatrix}
\dot{\vec{c}}_+(\tau) \\
\dot{\vec{c}}_-(\tau)
\end{bmatrix}
\rightarrow_{T \to \infty}
\begin{bmatrix}
1 \\
0
\end{bmatrix} =
\begin{bmatrix}
\vec{c}^A_+(\tau) \\
\vec{c}^A_-(\tau)
\end{bmatrix}
\] (32)

The difference between (30) and (31) is small, but rapidly oscillates with the dimensionless time \( \tau \). Therefore, it’s to be expected that the derivative with \( \tau \) of the difference is no longer small. In fact, letting \( F \equiv \sqrt{(\varepsilon T/\hbar)^2 + \pi^2} \), we have
\[
\begin{bmatrix}
\frac{d}{d\tau}\dot{\vec{c}}_+(\tau) \\
\frac{d}{d\tau}\dot{\vec{c}}_-(\tau)
\end{bmatrix}
\rightarrow_{T \to \infty}
\begin{bmatrix}
0 \\
i\pi e^{-i2\varepsilon T/\hbar}
\end{bmatrix} \neq \begin{bmatrix}
0 \\
0
\end{bmatrix} =
\begin{bmatrix}
\frac{d}{d\tau}\vec{c}^A_+(\tau) \\
\frac{d}{d\tau}\vec{c}^A_-(\tau)
\end{bmatrix}
\] (33)

**0.5 conclusion**

The above discussion shows: (i) The adiabatic state-vector \( \psi^A(t) \) does not satisfies approximately the Schrödinger differential equation, but it satisfies approximately the equivalent integral equation. (ii) The QAT is completely correct physically. This is ensured by \( \| \psi(t) - \psi^A(t) \| \ll 1 \). But it’s not necessarily true that \( \| \dot{\psi}(t) - \dot{\psi}^A(t) \| \ll 1 \). (iii) Taking \( \psi^A(t) \) for \( \dot{\psi}(t) \) will probably lead to contradiction.

Even though we don’t agree with [6], we still think it’s an interesting work. Because it has raised an important question: In theoretical reasoning, one has to bear in mind that approximately equal functions do not have to have approximately equal derivatives.

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**References**


